B.I.A.G.R.A.

BIbliotecA de proGRamación científicA

DEVEL

José Ángel de Bustos Pérez
<jadebustos@gmail.com>

Version RC 2.0, January 9, 2017.

LaTeX 2_ε

DEVEL

Contents

Preface

This library was created when I was studying my degree to ease my academic tasks when I was not forced to use Mathematica, Matlab, SPSS, Linpro, AN-SYS, Statgraphics, . . .

B.I.A.G.R.A stands for **BI**bliotec**A** de pro**GR**amación científic**A** which means Scientific Programming Library.

About the name? Well, for those days a new medicine was introduced into the market, my mind . . .

First version was *"published"* in 1998 but it is was not widely distributed.

Some months ago I started reviewing my backups to centralize useful stuff into only one repository and I found this library. Unfortunately the version I found was one of the first versions so a lot of stuff is missing:

- Matrix operations.

- Matrix factorization.

- System linear equations.

- Partial differential equations.

- . . .

This library was originally written in Spanish so I decided to translate into English and making it public available on Github.

It is important to remark that this release candidate version has not been tested and the results maybe not accurate enough. I will check and add tests to check it in a not distant future.

Today there are a lot of resources in many programming languages but in the days this library was published there was no much stuff available due to access to the internet was not as generalized as nowadays.

If you want to know how to use C language for scientific programming this code could be useful, specially how pointers are used to optimize memory usage and how function's pointers are used to abstact C functions from the mathematical functions they are going to use.

You can also check how to use threads using **OpenMP** and how to use the **GNU Multiple Precision Arithmetic Libary (GMP)**.

I will also add some code I created to test how a Fujitsu Primergy server scaled using Pi digits calculations.

I do not have any plans to increase this library. If I find the missing code I will add it though.

It is possible that I add some code from time to time due to the possibility I have to code some numerical methods in the future.

I hope this code is useful for you.

José Ángel de Bustos Pérez

License

This code is distributed under the GPLv2 License.

The author will be deeply grateful if this code is not used to:

- Attempt World domination.

- Use as compiling massive weapon.

- Translate it into Klingon.

- Ask for /home nationalisms.

- Reverse spelling it.

Just joking!!! Of course you can reverse spelling it (do you dare?).

José Ángel de Bustos Pérez

9

DEVEL

Chapter 1

What is *B.I.A.G.R.A* ?

- *B.I.A.G.R.A* stands for **BI***bliotec***A** *de pro***GR***amación científic***A** which means Scientific Programming Library.

- *B.I.A.G.R.A* is enterely coded using **C** language.

- *B.I.A.G.R.A* has been developed and tested under *LiNUX*.

- *B.I.A.G.R.A* is distribuded as open source and its author does not take any responibility.

- I wrote *B.I.A.G.R.A* in the 90s to help me with some academic tasks when studying my degree.

1.1   C language?

C language instead of **FORTRAN**?

- **C** is modular and structured.

- **C** is a general purpose language programming.

- **C** is a very powerful language and its code is very fast.

- **C** allows dynamic memory allocation.

- **C** code is portable.

- **C** is able to handle graphic modes.

1.2   Some general ideas about *B.I.A.G.R.A*

B.I.A.G.R.A has been developed under **Linux** and some **Linux** knowledge is needed.

B.I.A.G.R.A was developed to solve general problems instead of particular ones. For instance, instead of writing a program to get the inverse of a 4x4 matrix and having to change the source code to get the inverse of a 5x5 matrix *B.I.A.G.R.A* was developed to allow to write programs to get the inverse of any matrix without having to change de sorce code.

To be able to do that *pointers* were used instead of using *arrays*.

When we talk about *vectors* we will be talking about a *pointer* using dynamic memory allocation. When we talk about matrices we will be talking about *pointer* to a *pointer* using dynamic memory allocation.

B.I.A.G.R.A uses some data structures to store data.

For common errors as:

- Errors in dynamic memory allocation.

- Division by zero.

- …

B.I.A.G.R.A uses its own constants to notify these errors (Chapter 2).

1.3   How to install *B.I.A.G.R.A* under LiNUX

To install *B.I.A.G.R.A* :

```
# make static
```

The following actions will take place:

- Header files will be copied to `/usr/include/biagra`.

- The library will be placed at `/usr/lib/libbiagra.a-X.Y.Z` and a symbolic link named `/usr/lib/libbiagra.a` will be created pointing to `/usr/lib/libbiagra.a-X.Y.Z`.

- Example files will be copied to `/usr/share/biagra-X.Y.Z`.

To uninstall *B.I.A.G.R.A* :

```
# make uninstall
```

DEVEL

Chapter 2

B.I.A.G.R.A constants (const.h)

2.1 Introduction

B.I.A.G.R.A includes its own constants to be used if needed.

These constants are defined in `const.h`

2.2 Mathematical constants

Table 2.1 shows the *B.I.A.G.R.A* 's mathematical constanst.

Constant	Name	Value
e	BIA_E	2.71828182845904523536029
π	BIA_PI	3.14159265358979323846264

Table 2.1: *B.I.A.G.R.A* mathematical constants.

2.3 Logical constants

The following logical constants are defined:

BIA_FALSE when a condition is not met.

BIA_TRUE when a condiction is met.

2.4   Error constants

The following error constants are defined:

BIA_ZERO_DIV division by zero.

BIA_MEM_ALLOC error in memory allocation.

Chapter 3

Memory allocation (resmem.h)

3.1   Introduction

B.I.A.G.R.A includes its own memory allocation functions which are defined in `resmem.h` file.

3.2   Vector's memory allocation

Some functions are provided to handle memory allocations for vectors.

3.2.1   `intPtMemAllocVec` function

This functions allocates memory for a vector of int.

The definition of this function:

```
double *intPtMemAllocVec(int intElements);
```

This function has only one argument, `intElements`, which is the dimension of the vector and a `int` pointer is returned.

3.2.2   `dblPtMemAllocVec` function

This functions allocates memory for a vector of doubles.

The definition of this function:

```
double *dblPtMemAllocVec(int intElements);
```

This function has only one argument, `intElements`, which is the dimension of the vector and a `double` pointer is returned.

3.3   Matrix memory allocation

Some functions are provided to handle memory allocations for vectors.

3.3.1   `dblPtMemAllocMat` function

This function allocates memory for a matrix of doubles.

The definition of this function:

```
double **dblPtMemAllocMat(int intRows, int intCols);
```

where:

intRows number of rows.

intCols number of columns.

3.3.2   `dblPtMemAllocUpperTrMat` function

This function allocates memory for a upper triangular square matrix.

The definition of this function:

```
double **dblPtMemAllocUpperTrMat(int intOrder);
```

This function has only one argument, `intOrder`, which is the order of the matrix and a `double` pointer to pointer is returned.

In a upper triangular square matrix all elements below the diagonal are zero:

$$\begin{pmatrix} a_{0,0} & a_{0,1} & a_{0,2} & a_{0,3} & a_{0,4} \\ 0 & a_{1,1} & a_{1,2} & a_{1,3} & a_{1,4} \\ 0 & 0 & a_{2,2} & a_{2,3} & a_{2,4} \\ 0 & 0 & 0 & a_{3,3} & a_{3,4} \\ 0 & 0 & 0 & 0 & a_{4,4} \end{pmatrix}$$

For `intOrder = 5`:

```
myMatrix = dbpPtMemAllocUpperTrMat(5);
```

and:

B.I.A.G.R.A   18

Pointer	# elements	First element	Last element
myMatrix[0]	5	0	4
myMatrix[1]	4	0	3
myMatrix[2]	3	0	2
myMatrix[3]	2	0	1
myMatrix[4]	1	0	0

so:

$$myMatrix[i][j] = *(*(myMatrix + i) + j) = \begin{cases} a_{i,j+i} & \forall\ i \leq j \\ \\ 0 & \forall\ i > j \end{cases}$$

3.3.3 dblPtMemAllocLowerTrMat function

This function allowcates memory for a lower triangular square matrix.

The definition of this function:

```
double **dblPtMemAllocLowerTrMat(int intOrder);
```

This function has only one argument, intOrder, which is the order of the matrix and a double pointer to pointer is returned.

In a lower triangular square matrix all elements above the diagonal are zero:

$$\begin{pmatrix} a_{0,0} & 0 & 0 & 0 & 0 \\ a_{1,0} & a_{1,1} & 0 & 0 & 0 \\ a_{2,0} & a_{2,1} & a_{2,2} & 0 & 0 \\ a_{3,0} & a_{3,1} & a_{3,2} & a_{3,3} & 0 \\ a_{4,0} & a_{4,1} & a_{4,2} & a_{4,3} & a_{4,4} \end{pmatrix}$$

For intOrder = 5:

```
myMatrix = dbpPtMemAllocLowerTrMat(5);
```

and:

Pointer	# elements	First element	Last element
myMatrix[0]	1	0	0
myMatrix[1]	2	0	1
myMatrix[2]	3	0	2
myMatrix[3]	4	0	3
myMatrix[4]	5	0	4

so:

$$myMatrix[i][j] = *(*(myMatrix + i) + j) = \begin{cases} a_{i,j} & \forall \; i \leq j \\ 0 & \forall \; i < j \end{cases}$$

3.4   Freeing memory

B.I.A.G.R.A includes its own functions to free memory.

3.4.1   `freeMemDblMat` function

This functions frees memory for a matrix of doubles.

The definition of this function:

```
 void freeMemDblMat(double **dblMatrix, int intRows);
```

where:

dblMatrix double array to gree memory.

intRows number of matrix rows.

3.4.2   `freeMemIntMat` function

This functions frees memory for a matrix of integers.

The definition of this function:

```
 void freeMemIntMat(int **intMatrix, int intRows);
```

where:

intMatrix integer array to gree memory.

intRows number of matrix rows.

Chapter 4

Pseudo random numbers (random.h)

4.1 Introduction

B.I.A.G.R.A includes its own functions to pseudo random number generation and they are defined in `random.h` file.

> This functions have not been tested to produce unpredictable sequences, so be careful when use them.

4.2 Pseudo random integer numbers

4.2.1 `intRandom` function

This function generates random integers.

The definition of this function:

```
int intRandom(int limit);
```

The pseudo random integer is placed in the interval $(-limit, limit)$.

> Before using this function **srand** must be used to initialize **rand**. You can use **srand((unsigned)time(NULL))**.

The pseudo random number is generated with the following formula:

$$\left[\frac{limit \cdot rand()}{RAND\_MAX + 1}\right] \in (-limit, limit)$$

Then randomly is choosed if the number is positive or negative using the above formula with $limit = 2$ and then taking modulus 2. If modulus is 1 then the number will be a negative one.

4.2.2   uintRandom **function**

This function generates random integers.

The definition of this function:

```
int uintRandom(int limit);
```

The pseudo random integer is placed in the interval $[0, limit)$.

*Before using this function **srand** must be used to initialize rand. You can use **srand((unsigned)time(NULL))**.*

The pseudo random number is generated with the following formula:

$$\left[\frac{limit \cdot rand()}{RAND\_MAX + 1}\right] \in [0, limit)$$

4.3   Pseudo random floating point numbers

4.3.1   dblRandom **function**

This function generates random floating point numbers.

The definition of this function:

```
int dblRandom(int limit);
```

The pseudo random floating point number is placed in the interval $(-limit, limit)$.

*Before using this function **srand** must be used to initialize rand. You can use **srand((unsigned)time(NULL))**.*

The pseudo random number is generated with the following formula:

$$\frac{limit \cdot rand()}{RAND\_MAX + 1} \in (-limit, limit)$$

Then randomly is choosed if the number is positive or negative using the above formula with $limit = 2$ and then taking modulus 2. If modulus is 1 then the number will be a negative one.

4.3.2   `udblRandom` function

This function generates random floating point numbers.

The definition of this function:

```
int udblRandom(int limit);
```

The pseudo random floating point number is placed in the interval $[0, limit)$.

> Before using this function **srand** must be used to initialize **rand**. You can use **srand((unsigned)time(NULL))**.

The pseudo random number is generated with the following formula:

$$\frac{limit \cdot rand()}{RAND\_MAX + 1} \in [0, limit)$$

DEVEL

Chapter 5

Complex numbers (complex.h)

5.1 Introduction

Functions to manage complex numbers are defined in complex.h file.

5.2 Data structures

Some data structures are defined in *B.I.A.G.R.A* to manage complex numbers.

5.2.1 biaComplex data structure

biaComplex data structure is defined in figure 7.1 where:

intDegree polynomial degree.

intRealRoots number of real roots (if any).

intCompRoots number of complex roots (if any).

dblCoef pointer to store polynomial coeficients.

```
typedef struct {
  double dblReal,
         dblImag;
  } biaComplex;
```

Figure 5.1: biaComplex data structure.

5.2.2 `biaPolar` **data structure**

This data structure is used to store data for root approximation. Data structure is defined in figure 9.1 where:

intNMI maximum number of iterations to get the root with a maximum error of *dblTol*.

intIte iterations used to get the root.

dblx0 initial approximation to get the root.

dblRoot root approximation.

dblTol maximum tolerance when calculating the root.

dblError error in root approximation. Difference between the las two root approximations.

```
typedef struct {
  double dblMod,
         dblArg;
  } biaPolar;
```

Figure 5.2: biaPolar data structure.

5.3 Arithmetical operations using complex numbers

5.3.1 `addComplex` **function**

This function adds two complex numbers.

The definition of this function:

```
void addComplex(biaComplex *ptCmplx1, biaComplex *ptCmplx2,
                biaComplex *ptRes);
```

where:

*ptCmplx1 first complex number to be added.

*ptCmplx2 second complex number to be added.

*ptRes result of the operation.

5.3.2 `subtractComplex` **function**

This function subtracts two complex numbers.

The definition of this function:

```
void subtractComplex(biaComplex *ptCmplx1, biaComplex *ptCmplx2,
                     biaComplex *ptRes);
```

where:

*ptCmplx1 complex number.

*ptCmplx2 complex number to be subtracted to the above.

*ptRes result of the operation.

5.3.3 `multiplyComplex` **function**

This function multiplies two complex numbers.

The definition of this function:

```
void multiplyComplex(biaComplex *ptCmplx1, biaComplex *ptCmplx2,
                     biaComplex *ptRes);
```

where:

ptCmplx1 first complex number to be multiplied.

ptCmplx2 second complex number to be multiplied.

ptRes result of the operation.

5.3.4 `divideComplex` **function**

This function divides one complex number by other:

$$\frac{a + b \cdot i}{c + d \cdot i} = (a + b \cdot i) \cdot (c + d \cdot i)^{-1}$$

The definition of this function:

```
int divideComplex(biaComplex *ptCmplx1, biaComplex *ptCmplx2,
                  biaComplex *ptRes);
```

where:

*ptCmplx1 complex number.

*ptCmplx2 complex number used as divisor.

*ptRes result of the operation.

The following codes are returned:

BIA_ZERO_DIV	Division by zero
BIA_TRUE	Success

5.3.5 `invSumComplex` **function**

This function gets the additive inverse of a complex number:

$$\forall \ z_1 \in \mathbb{C} \quad \exists \ z_2 \in \mathbb{C} \ | \ z_1 + z_2 = 0$$

The definition of this function:

```
void invSumComplex(biaComplex *ptCmplx, biaComplex *ptRes);
```

where:

*ptCmplx complex number to get its additive inverse.

*ptRes where the additive inverse will be stored.

5.3.6 `invMulComplex` **function**

This function gets the multiplicative inverse of a complex number:

$$\forall \ z_1 \in \mathbb{C} - \{0\} = \mathbb{C}^* \quad \exists \ z_2 \in \mathbb{C} \ | \ z_1 \cdot z_2 = 1$$

The definition of this function:

```
int invMulComplex(biaComplex *ptCmplx, biaComplex *ptRes) ;
```

where:

*ptCmplx complex number to get its multiplicative inverse.

*ptRes where the additive multiplicative will be stored.

The following codes are returned:

BIA_ZERO_DIV	Division by zero
BIA_TRUE	Success

5.4   Complex number operations

5.4.1   `dblComplexModulus` function

This function gets the modulus of a complex number.

The definition of this function:

`double dblComplexModule(biaComplex *ptCmplx);`

where:

*ptCmplx complex number to get its modulus.

This function returns the complex number modulus.

5.4.2   `dblComplexArg` function

This function gets the argument of a complex number.

The definition of this function:

`double dblComplexArg(biaComplex *ptCmplx);`

where:

*ptCmplx complex number to get its argument.

This function returns the complex number argument (radians).

5.4.3   `conjugateComplex` function

This function gets the conjugate complex of a complex number:

$$z = a + b \cdot i \ \ \in \mathbb{C} \Rightarrow \overline{z} = a - b \cdot i \ \ \in \mathbb{C}$$

The definition of this function:

`void conjugateComplex(biaComplex *ptCmplx, biaComplex *ptRes);`

where:

*ptCmplx complex number to get its conjugate.

*ptRes complex conjugate.

5.4.4 `complex2Polar` **function**

This function gets the polar coordinates of a complex number.

The definition of this function:

```
void complex2Polar(biaComplex *ptCmplx, biaPolar *ptRes);
```

where:

*ptCmplx complex number to calculate polar coordinates.

*ptRes polar coordinates.

5.4.5 `polar2Complex` **function**

This function gets the cartesian coordinates of a polar coordinates for a complex number.

The definition of this function:

```
void polar2Complex(biaPolar *ptPolar, biaComplex *ptRes);
```

where:

*ptPolar polar coordinates.

*ptRes complex number in cartesian coordinates.

Argument is supposed to be in radians.

Chapter 6

Integer numbers (integers.h)

6.1 Introduction

B.I.A.G.R.A includes functions about integer numbers in `integers.h` file.

6.2 Sum integers

6.2.1 `uintSumFirstNIntegers` function

This function gets the sum of the first n integers.

The definition of this function:

`unsigned uintSumFirstNIntegers(int n);`

If the sum is bigger than an unsigned int 0 is returned.

6.3 Prime numbers

6.3.1 `isPrime` function

This function checks if a number is a prime number.

The definition of this function:

`int isPrime(int intN);`

The following codes are returned:

BIA_FALSE	`intN` is not a prime number
BIA_TRUE	`intN` is a prime number

31

6.3.2   `getFirstNPrimes` **function**

This function checks if a number is a prime number.

The definition of this function:

`void getFirstNPrimes(unsigned int *ptPrimes, int intNumber, int *ptCalc);`

where:

*ptPrimes array where primes will be stored. Memory allocation for this array has to be initialized before using this function.

intNumber number of primes to be computed.

*ptCalc in this variable the total amount of computed primes will be stored.

6.4   General

6.4.1   `uliFactorial` **function**

This function returns a integer's factorial.

The definition of this function:

`unsigned long int uliFactorial(int intN);`

where:

intN is the integer the factorial is going to be computed.

Factorial es returned as an `unsigned long int`.

Chapter 7

Polynomial (polynomials.h)

7.1   Introduction

Functions to manage polynomials are defined in polynomial.h file.

A polynomial used to be represented as shown in equation 7.1.

$$p(x) = a_0 + a_1 \cdot x + \cdots + a_n \cdot x^n = \sum_{i=0}^{n} a_i \cdot x^i \qquad \text{where } a_i \in \mathbb{R} \qquad (7.1)$$

7.2   Data structures

Some data structures are defined in $B.I.A.G.R.A$ to manage polynomials.

7.2.1   biaRealPol data structure

This data structure is used to handle polinomials $p(x) \in \mathbb{R}[x]$. **biaPol** data structure is defined in figure 7.1 where:

intDegree polynomial degree.

intRealRoots number of real roots (if any).

intCompRoots number of complex roots (if any).

dblCoefs pointer to store polynomial coeficients.

dblRoots pointer to store real polynomial roots.

```
typedef struct {
  int  intDegree   = 0,
       intRealRoots = 0,
       intCompRoots = 0;

  double  *dblCoefs,
          *dblRoots;
  } biaRealPol;
```

Figure 7.1: biaRealPol data structure.

Polynomial coeficients are stored in `dblCoefs` pointer which has to be previously initialized:

$$\begin{aligned}
\text{dblCoefs}[0] &= a_0 \\
\text{dblCoefs}[1] &= a_1 \\
&\ldots \ldots \ldots \\
\text{dblCoefs}[n] &= a_n
\end{aligned}$$

dblRoots are stored in the same way as dblCoefs.

7.3   Polynomials operations

7.3.1   addPol function

This function adds two polynomials.

The definition of this function:

```
int addPol(biaPol *ptPol1, biaPol *ptPol2, biaPol *ptRes);
```

where:

ptPol1 pointer to a `biaRealPol` struct with the first polynomial to be added.

ptPol2 pointer to a `biaRealPol` struct with the second polynomial to be added.

ptRes pointer to a `biaRealPol` struct where the add operation will be stored.

The following codes are returned:

BIA_MEM_ALLOC	Memory allocation error
BIA_TRUE	Success

> *ptRes* *will be released and memory allocation will be carried out to store the derivative.*

> *ptRes* *member* *dblCoefs* *has to be initialized to a* *NULL* *pointer to avoid a* **Segment Fault** *error if it was not previously initialized.*

7.3.2   dblEvaluatePol **function**

This function returns the polynomial value in a given point.

The definition of this function:

`double dblEvaluatePol(biaRealPol *ptPol, double dblX);`

where:

ptPol pointer to a `biaRealPol` struct with the polynomial to be evaluated.

dblX value in which the polynomial will be evaluated.

> *Polynomial is defined over* $\mathbb{R}[x]$.

7.3.3   derivativePol **function**

This function gets the n-th derivative of a polynomial.

The definition of this function:

`int derivativePol(biaPol *ptPol, biaPol *ptDer, int intN);`

where:

ptPol pointer to a `biaRealPol` struct with the polynomial to get its derivative is stored.

ptDer pointer to a `biaRealPol` struct where the derivative will be stored.

intN order of the derivative to get.

The following codes are returned:

BIA_MEM_ALLOC	Memory allocation error
BIA_TRUE	Success

ptDer will be released and memory allocation will be carried out to store the derivative.

ptDer member *dblCoefs* has to be initialized to a *NULL* pointer to avoid a **Segment Fault** error if it was not previously initialized.

7.3.4   `multiplyPol` function

This functions multiplies two polynomials.

The definition of this function:

```
int multiplyPol(biaPol *ptPol1, biaPol *ptPol2, biaPol *ptRes);
```

where:

ptPol1 pointer to a `biaRealPol` struct with the first polynomial.

ptPol2 pointer to a `biaRealPol` struct with the second polynomial.

ptRes pointer to a `biaRealPol` struct where the multiplication operation will be stored.

The following codes are returned:

BIA_MEM_ALLOC	Memory allocation error
BIA_TRUE	Success

ptRes *will be released and memory allocation will be carried out to store the derivative.*

ptRes *member* `dblCoefs` *has to be initialized to a* `NULL` *pointer to avoid a* **Segment Fault** *error if it was not previously initialized.*

7.3.5 `polFromRealRoots` **function**

This function get the polynomial expression from its real roots.

The definition of this function:

`int polFromRealRoots(double *dblRoots, int intNumber, biaRealPol *ptPol);`

where:

dblRoots pointer to a `double` with the polynomial real roots.

intNumber number or real roots.

ptPol pointer to a `biaRealPol` struct where the polynomial will be stored.

The following codes are returned:

BIA_MEM_ALLOC	Memory allocation error
BIA_TRUE	Success

intNumber *includes roots multiplicity so* *intNumber* *is equal to polynomial degree.*

Each polynomial root must be included as many times as its multiplicity.

7.3.6 `subtractPol` **function**

This function subtracts two polynomials.

The definition of this function:

`int subtractPol(biaPol *ptPol1, biaPol *ptPol2, biaPol *ptRes);`

where:

ptPol1 pointer to a `biaRealPol` struct with the first polynomial.

ptPol2 pointer to a `biaRealPol` struct with the polynomial to be subtracted from the above.

ptRes pointer to a `biaRealPol` struct where the subtract operation will be stored.

The following codes are returned:

BIA_MEM_ALLOC	Memory allocation error
BIA_TRUE	Success

ptRes will be released and memory allocation will be carried out to store the derivative.

ptRes member *dblCoefs* has to be initialized to a *NULL* pointer to avoid a **Segment Fault** error if it was not previously initialized.

Chapter 8

Matrix (matrix.h)

8.1 Introduction

Functions to manage matrices are defined in matrix.h file.

8.2 Data structures

Some data structures are defined in *B.I.A.G.R.A* to manage matrices.

8.2.1 biaMatrix data structure

This data structure is used to store a matrix. **biaMatrix** data structure is defined in figure 8.1 where:

intRows number of rows.

intCols number of columns.

dblCoefs pointer to store matrix coeficients.

```
typedef struct {
  int intRows,
      intCols;

  double **dblCoefs;
  } biaMatrix;
```

Figure 8.1: biaMatrix data structure.

8.3 Matrix creation

B.I.A.G.R.A includes functions to create some kind of matrices.

8.3.1 `identityMatrix` function

This function stores the identity matrix with order taken from intRows member of `ptMatrix`:

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & \ddots & 0 & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & \ddots & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

The definition of this function:

```
void identityMatrix(biaMatrix *ptMatrix);
```

where:

*ptMatrix matrix that has to be created before using this function. Memory allocation for `dblCoefs` must be done before using this function.

intRows is used to get the matrix order.

8.3.2   `scalingMatrix` **function**

This function stores the scaling matrix with factor λ and order taken from intRows member of `ptMatrix`:

$$\begin{pmatrix} \lambda & 0 & 0 & 0 & 0 \\ 0 & \lambda & \ddots & 0 & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & \ddots & \lambda & 0 \\ 0 & 0 & 0 & 0 & \lambda \end{pmatrix}$$

The definition of this function:

`void scalingMatrix(biaMatrix *ptMatrix, double dblFactor);`

where:

*ptMatrix matrix that has to be created before using this function. Memory allocation for `dblCoefs` must be done before using this function.

> *intRows* *is used to get the matrix order.*

8.3.3   `nullMatrix` **function**

This function stores the null matrix with order taken from intRows member of `ptMatrix`:

$$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \ddots & 0 & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & \ddots & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

The definition of this function:

`void nullMatrix(biaMatrix *ptMatrix);`

where:

*ptMatrix matrix that has to be created before using this function. Memory allocation for `dblCoefs` must be done before using this function.

> *intRows* and *intCols* is used to get the matrix order.

8.4 Matrix operations

8.4.1 transposeMatrix **function**

This function stores the transpose matrix of a given matrix.

The definition of this function:

```
void transposeMatrix(biaMatrix *ptMatrix, biaMatrix *ptRes);
```

where:

*ptMatrix matrix to get its transpose matrix.

*ptRes matrix to store the transpose matrix. Memory has to be preallocated before using this function.

> *intRows* and *intCols* is used to get the matrix order.

8.5 Matrix checks

8.5.1 isIdentityMatrix **function**

This function checks if a matrix is the identity matrix.

The definition of this function:

```
int isIdentityMatrix(biaMatrix *ptMatrix);
```

where:

*ptMatrix matrix to check.

8.5.2 `isNullMatrix` **function**

This function checks if a matrix is a null matrix.

The definition of this function:

`int isNullMatrix(biaMatrix *ptMatrix, double dblTol);`

where:

*ptMatrix matrix to check.

dblTol if a matrix element is minor than this value it is assumed it is a null element.

8.5.3 `isSymmetricMatrix` **function**

This function checks if a matrix is a symmetric matrix.

The definition of this function:

`int isSymmetricMatrix(biaMatrix *ptMatrix);`

where:

*ptMatrix matrix to check.

DEVEL

Chapter 9

Roots approximation (roots.h)

9.1 Introduction

Functions to compute function's roots approximation are defined in `roots.h` file.

9.2 Data structures

Some data structures are defined in *B.I.A.G.R.A* to manage roots.

9.2.1 `biaRealRoot` data structure

This data structure is used to store data for root approximation.

Data structure is defined in figure 9.1 where:

intNMI maximum number of iterations to get the root with a maximum error of `dblTol`.

intIte iterations used to get the root.

dblx0 initial approximation to get the root.

dblRoot root approximation.

dblTol maximum tolerance when calculating the root.

dblError error in root approximation. Difference between the las two root approximations.

```
typedef struct {
  int intNMI,
      intIte;

  double dblx0,
         dblRoot,
         dblTol,
         dblError;
  } biaRealRoot;
```

Figure 9.1: biaRealRoot data structure.

9.3   Function roots approximation

9.3.1   `newtonPol` function

This function approaches a polynomial root using the **Newton** method.

The definition of this function:

`int newtonPol(biaPol *ptPol, biaRealRoot *ptRoot);`

The following codes are returned:

BIA_MEM_ALLOC	Memory allocation error
BIA_ZERO_DIV	Division by zero
BIA_TRUE	the root was computed satisfying the problem conditions (`intMNI` and `dblTol`);
BIA_FALSE	Root approximation could not be calculated satisfying the requirements (`intMNI` and `dblTol`).

The following values in `*ptRoot` need to be initialized:

intMNI maximun number of iterations to compute the root.

dblx0 initial approximation.

dblTol tolerance to compute de root.

The following data will be stored:

intIte iterations used to compute the root.

dblRoot approximation of the root.

dblError error in the approximation.

> *When two consecutive approximations are close enough,* `dblTol`, *last approximation will be considered as good and will be stored in* `*biaRealRoot *ptRoot` *in* `dblRoot`.

9.3.2 `newtonMethod` **function**

This function approaches a function's root using the **Newton** method.

The definition of this function:

```
int newtonMethod(biaRealRoot *ptRoot,
      int (*func)(double dblx0, double *ptRes),
      int (*der)(double dblx0, double *ptRes));
```

Function's pointers are used to avoid having to recode the C function every time a root function need to be approximated for different mathematical functions.

The following codes are returned:

BIA_ZERO_DIV	Division by zero
BIA_TRUE	the root was computed satisfying the problem conditions (`intMNI` and `dblTol`);
BIA_FALSE	Root approximation could not be calculated satisfying the requirements (`intMNI` and `dblTol`).

where:

ptRoot is a pointer to a `biaRealRoot` variable.

func pointer to a function implementing the function which root is going to be computed.

der pointer to a function implementing the derivative of the function which root is going to be computed.

The following values in *ptRoot need to be initialized:

intMNI maximun number of iterations to compute the root.

dblx0 initial approximation.

dblTol tolerance to compute de root.

The following data is stored:

intIte iterations used to compute the root.

dblRoot approximation of the root.

dblError error in the approximation.

> *When two consecutive approximations are close enough,* `dblTol`*, last approximation will be considered as good and will be stored in* `*biaRealRoot *ptRoot` *in* `dblRoot`*.*

Usage example

To approximate a root for the function $f(x) = \sqrt{2}$ to C functions need to be created. A C function for the mathematical function implementation:

```
/* f(x) = x^2 - 2 */
int myfunc(double x0, double *fx0) {
  *fx0 = (double)(x0 * x0 - 2.);
  return BIA_TRUE;
}
```

A C function for the mathematical derivative function implementation:

```
/* f'(x) = 2*x */
int myfuncder(double x0, double *fx0) {
  *fx0 = 2.*x0;
  return BIA_TRUE;
}
```

Both functions must meet the following requirements:

- An integer value is returned, **BIA_TRUE** when function is evaluated in $x0$ and **BIA_ZERO_DIV** if a division by zero takes place.

- $x0$ value to evaluate the function.

- $*fx0$ pointer to a double to store the function's value in $x0$.

So to approximate function's root using Newton Method:

```
i = newtonMethod(&myRoot, &myfunc, &myfuncder);
```

Chapter 10

Runge-Kutta methods (rngkutta.h)

10.1 Introduction

Runge-Kutta are a family of implicit and explicit iterative methods used to approximate solutions of ordinary differential equations or **ODE**.

Butcher matricial notation is used in this implementation.

10.2 Data structures

10.2.1 `biaButcherArray` data structure

This structure is used to store the Butcher matricial notation.

Data structure is defined in figure 10.1 where:

intStages method stages.

*dblC c_i coefficients stored in an array with size `intStages`.

*dblB b_i coefficients stored in an array with size `intStages`.

**dblMatrix matrix to store $a_{i,j}$ method's coeficients.

```
typedef struct {
  double  *dblC,
          *dblB,
          **dblMatrix;

  int     intStages;
} biaButcherArray;
```

Figure 10.1: biaButcherArray data structure.

> *See appendix A if you need information about Butcher matricial notation.*

10.2.2   biaDataRK **data structure**

This structure is used to store all the data needed to apply a Runge-Kutta method.

Data structure is defined in figure 10.2 where:

intNumApprox number of approximations to be done (size of the array dblPoints).

intImplicit when the Runge-Kutta method is implicit or not. The following constants are defined in the header file:

Name	Value
BIA_IMPLICIT_RK_TRUE	0
BIA_IMPLICIT_RK_FALSE	1

*dblPoints array with dimension intNumApprox and its elements will be the approximations in x_i where:

$$x_i = dblFirst + i \cdot dblStepSize \qquad \text{where} \qquad 0 \leq i < intNumApprox$$

dblStepSize method's step-size.

dblFirst first point used to compute all the approximations. The value of the function in this point is known (initial condition).

dblLast last point in which approximations will be computed.

strCoefs variable of type biaButcherArray (section 10.2.1) storing Butcher
matricial notation.

```
typedef struct {
  int intNumApprox,
      intImplicit;

  double  *dblPoints,
          dblStepSize,
          dblFirst,
          dblLast;

  biaButcherArray strCoefs;
} biaDataRK;
```

Figure 10.2: biaDataRK data structure.

10.3   Node number calculations

10.3.1   intNodeNumber function

This function gets the number of nodes that can be placed in an interval. All
nodes are equidistant.

The definition of this function:

`int intNodeNumber(double dblLong, double dblStepSize)`

where:

dblLong interval length.

dblStepSize distance between two nodes.

The function returns the number of nodes that can be placed.

Arguments are supposed to be different from zero.

Arguments are supposed to be positive.

10.4   Explicit Runge-Kutta methods (scalar problems)

10.4.1   `explicitRungeKutta` function

This function solves an *I.V.P.* using an explicit Runge-Kutta method.

The definition of this function:

```
int explicitRungeKutta(biaDataRK *ptData,
                double (*IVP)(double dblX, double dblY)
```

where:

ptData pointer to a **biaDataRK** variable[1]. This variable contains all the necessary data to solve the *I.V.P.*

IVP C function's pointer to a function implementing the *O.D.E.*. This functions needs to have two double arguments and returns the value of the *I.V.P.*:

   dblX point where we want to evaluate the *O.D.E.*

   dblY *O.D.E.* value in `dblX` ($y_i \approx y(x_i)$).

The following codes are returned:

BIA_MEM_ALLOC	Memory error allocation
BIA_TRUE	Success

Usage example

For instance, to solve this *I.V.P.*:

$$\begin{cases} y' = y(x) * \frac{x - y(x)}{x^2} \\ y(1) = 2 \end{cases}$$

the implementation of the `IVP` would be:

```
double IVP(double dblX, double dblY) {
  double  dblResultado;

  dblRes = dblY*((dblX-dblY)/(dblX*dblX));

  return (dblRes);
}
```

---

[1]Section (10.2.2).

A `biaDataRK` variable has to be initialized. *B.I.A.G.R.A* provides several functions to initialize the `biaButcherArray` member.

To solve the *I.V.P.* problem:

```
i = explicitRungeKutta(&varDataRK, IVP);
```

10.4.2 `classicRungeKuttaCoefs` function

This function initialize the Butcher array for the classic Runge-Kutta method (four-stage method and order two).

The definition of this function:

```
int classicRungeKuttaCoefs(biaDataRK *ptData);
```

where:

ptData pointer to a **biaDataRK** variable[2]. In this variable the following members will be initialized:

intStages will be initialized to 4.

intImplicit will be initialized to BIA_IMPLICIT_RK_FALSE.

strCoefs will be initialized with the Butcher array.

The Butcher array for this method:

$$
\begin{array}{c|cccc}
0 & 0 \\
\frac{1}{2} & \frac{1}{2} & 0 \\
\frac{1}{2} & 0 & \frac{1}{2} & 0 \\
1 & 0 & 0 & 1 & 0 \\
\hline
 & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6}
\end{array}
$$

The following codes are returned:

BIA_MEM_ALLOC	Memory error allocation
BIA_TRUE	Success

---

[2]Section (10.2.2).

10.4.3 `heunRungeKuttaCoefs` function

This function initialize the Butcher array for the Heun Runge-Kutta method
(three-stage method and order three).

The definition of this function:

`int heunRungeKuttaCoefs(biaDataRK *ptData);`

where:

ptData pointer to a **biaDataRK** variable[3]. In this variable the following
members will be initialized:

intStages will be initialized to 3.

intImplicit will be initialized to BIA_IMPLICIT_RK_FALSE.

strCoefs will be initialized with the Butcher array.

The Butcher array for this method:

$$
\begin{array}{c|ccc}
0 & 0 & & \\
\frac{1}{3} & \frac{1}{3} & 0 & \\
\frac{2}{3} & 0 & \frac{2}{3} & 0 \\
\hline
& \frac{1}{4} & 0 & \frac{3}{4}
\end{array}
$$

The following codes are returned:

BIA_MEM_ALLOC	Memory error allocation
BIA_TRUE	Success

10.4.4 `kuttaRungeKuttaCoefs` function

This function initialize the Butcher array for the Kutta Runge-Kutta method
(three-stage method and order three).

The definition of this function:

`int kuttaRungeKuttaCoefs(biaDataRK *ptData);`

where:

ptData pointer to a **biaDataRK** variable[4]. In this variable the following
members will be initialized:

---

[3]Section (10.2.2).

[4]Section (10.2.2).

intStages will be initialized to 3.

intImplicit will be initialized to BIA_IMPLICIT_RK_FALSE.

strCoefs will be initialized with the Butcher array.

The Butcher array for this method:

$$
\begin{array}{c|ccc}
0 & 0 & & \\
\frac{1}{2} & \frac{1}{2} & 0 & \\
1 & -1 & 2 & 0 \\
\hline
 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6}
\end{array}
$$

The following codes are returned:

BIA_MEM_ALLOC	Memory error allocation
BIA_TRUE	Success

10.4.5 modifiedEulerRungeKuttaCoefs function

This function initialize the Butcher array for the modified Euler Kutta Runge-Kutta method (two-stage method and order two).

The definition of this function:

`int modifiedEulerRungeKuttaCoefs(biaDataRK *ptData);`

where:

ptData pointer to a **biaDataRK** variable[5]. In this variable the following members will be initialized:

intStages will be initialized to 2.

intImplicit will be initialized to BIA_IMPLICIT_RK_FALSE.

strCoefs will be initialized with the Butcher array.

The Butcher array for this method:

$$
\begin{array}{c|cc}
0 & 0 & \\
\frac{1}{2} & \frac{1}{2} & 0 \\
\hline
 & 0 & 1
\end{array}
$$

The following codes are returned:

BIA_MEM_ALLOC	Memory error allocation
BIA_TRUE	Success

[5]Section (10.2.2).

10.4.6   `improvedEulerRungeKuttaCoefs` function

This function initialize the Butcher array for the improved Euler Runge-Kutta method (two-stage method and order two).

The definition of this function:

`int improvedRungeKuttaCoefs(biaDataRK *ptData);`

where:

ptData pointer to a **biaDataRK** variable[6]. In this variable the following members will be initialized:

> **intStages** will be initialized to 3.
>
> **intImplicit** will be initialized to BIA_IMPLICIT_RK_FALSE.
>
> **strCoefs** will be initialized with the Butcher array.

The Butcher array for this method:

$$
\begin{array}{c|cc}
0 & 0 & \\
1 & 1 & 0 \\
\hline
 & \frac{1}{2} & \frac{1}{2}
\end{array}
$$

The following codes are returned:

BIA_MEM_ALLOC	Memory error allocation
BIA_TRUE	Success

---

[6]Section (10.2.2).

Chapter 11

Numerical integration (numintegr.h)

11.1 Introduction

In this chapter numerical methods to compute defined integrals will be defined.

The following libraries will be used:

- OpenMP the Open Multi Processing API which provides multiplatform shared memory capabilities for parallel programming.

11.2 The midpoint rule (threaded version)

This implementation of the midpoint rule is a multithreaded implementation using OpemMP.

Using n subintervals the midpoint rule:

$$\int_a^b f(x)dx \approx \sum_{i=0}^{n-1} f(\frac{1}{2} \cdot (x_i + x_{i+i})) \triangle x \quad \text{where} \quad \triangle x = \frac{b-a}{n}$$

11.2.1 `threadedMidPointRule` function

This function uses a threaded version of the midpoint rule to compute an integral over an inteval.

The definition of this function:

```
long double threadedMidPointRule(int intThreads, int intN,
          double a, double b, long double (*func)(double x));
```

where:

intThreads number of threads to be used.

intN number of subintervals to be used.

a Interval left endpoint.

b Interval right endpoint.

func C function's pointer to a function implementing the function we want
to compute the integral. This function needs to have one long double
argument and returns the function's value in the argument point (as
long double).

Usage example

To compute:

$$\int_0^1 \frac{1}{1+x^2} dx$$

the implementation of the **func** would be:

```
long double func(double x) {
  return (1/(1+(x*x)));
}
```

and to compute it using 4 threads an 15000 subintervals:

```
value = threadedMidPointRule(4, 15000, 0., 1., &func);
```

Chapter 12

π computation (pi.h)

12.1 Introduction

In this chapter several methods will be shown to compute π digits.

The following libraries will be used:

- OpenMP the Open Multi-Processing API which provides multiplatform shared memory capabilities for parallel programming.

- GMP the GNU Multiple Precision Arithmetic Library.

12.2 The midpoint rule method

To compute π value using the midpoint rule the following is used:

$$\int_0^1 \frac{1}{1+x^2}dx = \frac{\pi}{4}$$

So:

$$\pi = 4 \cdot \int_0^1 \frac{1}{1+x^2}dx$$

12.2.1 `threadedPiMidPointRule` function

This function approaches π using the midpoint rule.

The definition of this function:

```
long double threadedPiMidPointRule(int intThreads, int intN);
```

where:

intThreads number of threads to be used.

intN number of subintervals to be used.

> *To compute the integral the midpoint rule will be used. The implementation used for the midpoint rule used is the one provided by* B.I.A.G.R.A *in section* 11.2.1.

12.3   Chudnovsky algorithm

The Chudnovsky algorithm uses the following to compute π:

$$\pi \cdot \sum_{i=0}^{\infty} \frac{(6 \cdot i)! \cdot (13591409 + 545140134 \cdot i)}{(3 \cdot i)! \cdot (i!)^3 \cdot (-640320)^{3 \cdot i}} = 426880 \cdot \sqrt{10005}$$

For high performance computation.

$$\pi \cdot \sum_{i=0}^{\infty} \frac{(6 \cdot i)! \cdot (13591409 + 545140134 \cdot i)}{(3 \cdot i)! \cdot (i!)^3 \cdot (-262537412640768000)^i} = 426880 \cdot \sqrt{10005}$$

12.3.1   `chudnovskyPi` function

This function approaches π using the Chudnovsky algorithm.

The definition of this function:

```
int chudnovskyPi(int intThreads, int intPiDigits, char *ptPi);
```

where:

intThreads number of threads to be used.

intPiDigits number of π digits to compute.

ptPi char point to store π as a string.

> *This algorithm uses the **GNU Multiple Precision Library (GMP)** to be able to perform all the computations. C default number types do not provide enough precision.*

> *This algorithm uses **OpenMP** to be able to parallelize computations.*

ptPi *must be initialized to store* π *as a string. For instance to store* 100 π *digits the size to allocate memory is* 102 *to include the ".” character and the “null character” at the end of the string.*

DEVEL

DEVEL

Part I

Appendices

Appendix A

Runge-Kutta methods introduction

This appendix is intended to help to know how Runge-Kutta methods are implemented and used in this library.

A.1   What is a Runge-Kutta method?

Runge-Kutta methods are a family of numerical methods to approach solutions of ordinary differential equations (O.D.E). These methods are iterative methods used to solve *"initial problem value"* (**I.P.V**) or *"Cauchy problem"*.

These methods are only-one-step methods with a fixed size for the method step[1].

A.1.1   What is a I.V.P.?

An *I.V.P.* is:

$$\begin{cases} y' = f(x, y(x)) \\ y(x_0) = y_0 \end{cases} \tag{A.1}$$

So y' is a function depending on the variable x, and the function $y(x)$. $y(x)$ is the solution of the equation A.1 and the point (x_0, y_0) belongs to the curve $y(x)$.

---

[1]It is also possible to implement methods with a variable step known as *embedding*.

Solving the *I.V.P.* A.1 is finding a function $y(x)$ such as the equation A.1 is met.

An example of a *I.V.P.*:

$$\begin{cases} y' = \frac{x*y(x)-y(x)^2}{x^2} \\ y(1) = 2 \end{cases} \tag{A.2}$$

The solution of the A.2 will be:

$$y(x) = \frac{x}{\frac{1}{2} + \ln x} \tag{A.3}$$

A.2   Runge-Kutta's method notation

$y(x_i)$ will be the exact value of the function $y(x)$ evaluated in x_i.

y_i will be the approximation of the function $y(x)$ in the point x_i.

h is the step used by the method in each iteration.

A.2.1   General formulation

A s-stages **Runge-Kutta**'s method formulation is:

$$y_{n+1} = y_n + h \cdot \sum_{i=0}^{s-1} b_i \cdot k_i \tag{A.4}$$

where:

$$k_i = f(x_n + c_i \cdot h, y_n + h \cdot \sum_{j=0}^{s-1} a_{i,j} \cdot k_j) \tag{A.5}$$

satisfying:

$$\sum_{j=0}^{s-1} a_{i,j} = c_i \tag{A.6}$$

A.2.2   Matricial notation (Butcher's)

Matricial notation is used to represent method's coeficients using a matrix.

For a s-stages **Runge-Kutta** method the matricial notation will be:

$$
\begin{array}{c|ccc}
c_0 & a_{0,0} & \cdots\cdots & a_{0,s-1} \\
\vdots & \vdots & & \vdots \\
\vdots & \vdots & & \vdots \\
c_{s-1} & a_{s-1,0} & \cdots\cdots & a_{s-1,s-1} \\
\hline
 & b_0 & \cdots\cdots & b_{s-1}
\end{array}
$$

In section 10.2.1 is shown a data structure used to store the Butcher array.

A.3   Runge-Kutta types

There are several types of **Runge-Kutta** methods.

A.3.1   Implicit Runge-Kutta

A **Runge-Kutta** method is said to be implicit when the $a_{i,j} \neq 0$ for some $j > i$.

The 2-stages Gauss method is an implicit **Runge-Kutta** method of 2-stages:

$$
\begin{array}{c|cc}
\frac{3-\sqrt{3}}{6} & \frac{1}{4} & \frac{3-2*\sqrt{3}}{12} \\
\frac{3+\sqrt{3}}{6} & \frac{3+2*\sqrt{3}}{12} & \frac{1}{4} \\
\hline
 & \frac{1}{2} & \frac{1}{2}
\end{array}
$$

A.3.2   Semi-implicit Runge-Kutta

A **Runge-Kutta** method is said to be semi-implicit when the $a_{i,j} = 0$ when $j > i$.

A 2-stages semi-implicit **Runge-Kutta** method:

$$
\begin{array}{c|cc}
\frac{3+\sqrt{3}}{6} & \frac{3+\sqrt{3}}{6} & 0 \\
\frac{3-\sqrt{3}}{6} & \frac{-\sqrt{3}}{3} & \frac{3+\sqrt{3}}{6} \\
\hline
 & \frac{1}{2} & \frac{1}{2}
\end{array}
$$

A.3.3   Explicit Runge-Kutta

A **Runge-Kutta** method is said to be explicit when the $a_{i,j} = 0$ when $j \geq i$.

A 4-stages explicit **Runge-Kutta** method also known as "**classic Runge-Kutta**":

$$
\begin{array}{c|cccc}
0 & 0 \\
\frac{1}{2} & \frac{1}{2} & 0 \\
\frac{1}{2} & 0 & \frac{1}{2} & 0 \\
1 & 0 & 0 & 1 & 0 \\
\hline
 & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6}
\end{array}
$$